

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 289 °C

Global applicability domain: Outside

Local applicability domain index: 1.34e-01

Confidence level: 5.97e-01

Nearest Neighbors from the Training Set

Image not found

Diphenylurea

Measured: 262

Predicted: 269

Image not found

Benzoic acid, 2-phenylhydrazide

Measured: 314

Predicted: 306

Image not found

N-(4-Bromophenyl)urea

Measured: 260

Predicted: 256

Image not found

2-Nitrobenzamide

Measured: 317

Predicted: 310

Image not found

2-Acetylaminofluorene

Measured: 303

Predicted: 340